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**Final Report for Grant NAG5-4381
from the NASA Planetary Atmospheres Program**

STUDIES OF TENUOUS PLANETARY ATMOSPHERES

**Research Area:
Composition/Structure/Dynamics of Comet and
Planetary Satellite Atmospheres**

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I. PROJECT OVERVIEW

I.A. Scientific Objectives In order to understand the physical and chemical processes which produce the tenuous planetary and planetary satellite (upper) atmospheres through interactions with their particle, field, and radiation environs, it is necessary analyze remotely observed and spacecraft data with physically meaningful models. With this in mind, we have undertaken a coupled program of theoretical modeling and complementary data analysis regarding the global distributions of neutral and ionized gases in, and escape from, tenuous planetary atmospheres of Io and Europa. The theoretical models developed will have further applications to other tenuous atmospheres such as that of Pluto and Titan or the upper atmospheres of the terrestrial planets.

I.B. Significance and Relevance This project addresses prime areas of study central to current and future NASA missions and for the goals of NASA's overall program in the study and exploration of the solar system and its origin. In the published report of COMPLEX, the Committee on Planetary and Lunar Exploration, of the Space Studies Board, National Research Council, comets and the Jupiter system were identified in the highest priority group.

Io and Europa, their atmospheres, and their interactions with Jupiter's plasma torus, are prominent in current and future NASA science goals and missions. A unique combination of modeling tools which have been, and continue to be, developed at the University of Michigan have already been applied to understand Galileo particle and fields measurements obtained during its encounters with Io and Europa. Both the Galileo mission and the Galileo Europa mission and remote measurements with the Hubble Space Telescope will continue to be sources of new results, as data already taken is reduced and released, and as upcoming encounters with Io and Europa yield new important insight into these atmospheres. NASA is developing plans for the Europa Orbiter mission for studying the icy surface and mantle below the icy surface, which may hold the clues to the thin extended atmosphere.

I.C. Strategy and Approach Our overall strategy is and has been to develop and apply sophisticated models of the type normally used in purely theoretical studies for the purpose of directly comparing models with measurements in order to gain a deeper understanding of the physical state and composition of the atmosphere in question. Typical first-principles theoretical

investigations produce many detailed calculations to explore the type and range of physical phenomena that might or should occur, but are often only loosely constrained by observed characteristics and are often limited to physically overly simplistic assumptions. On the other hand, typical measurements, whether Earth-based and near-Earth based remote observations, or *in situ* spacecraft measurements, are often limited to fairly simple model analyses (scale-height distributions, uniform columns, constant temperatures, simple imposed uniform magnetic fields, etc.). The PI's approach throughout his studies with collaborators dealing both with comets and satellite atmospheres has been to use physically meaningful models and compare directly with data. For this reason we have developed the core modeling tools, and either analyze published measurements, or establish various collaborations with observers. The subjects of study covered here are unified by this overarching strategy.

II. Progress Report

Work under this grant has lead to publication of two papers on the MHD modeling of the interaction of the plasma torus with Io (Combi et al. 1998; Kabin et al. 2000), two papers on the MHD modeling of the interaction of the plasma torus with Europa (Kabin et al. 1999; Liu et al. 2000), a review paper on a large set of MHD model results, (Kabin et al. 2000), and the writing and submission of a refereed review paper for a special AGU monograph on the comparative aspects of tenuous cometary and planetary satellite atmospheres/ionospheres and their interactions with their outer particles and fields environs—either planetary magnetosphere or solar wind (Combi, Gombosi and Kabin 2002). In addition, some of the ion particle-pushing algorithms included in our kinetic DSMC model were described in a paper on the transport of particles from the impact site of comet Shoemaker-Levy 9 on Jupiter to the conjugate hemisphere (Bauske, Combi and Clarke 2000). Dr. Konstantin Kabin, obtained his Ph.D. in 2000 (Kabin 2000) with much of his support from this grant.

Refereed publications describing work supported by this grant are:

- 1) *Combi, M.R., K. Kabin, T.I. Gombosi, D.L. DeZeeuw, K.G. Powell. Io's Plasma Environment during the Galileo Flyby: Global Three-Dimensional MHD Modeling with Adaptive Mesh Refinement. J. Geophys. Res. 103 (A5), 9071-9081 1998.*

- 2) Bauske, R., M.R. Combi, J.T. Clarke. *Analysis of Mid-Latitude Auroral Emissions Observed During the Impact of Comet Shoemaker-Levy 9 With Jupiter. Icarus* **142**, 106-115, 1999.
- 3) Kabin, K., M.R. Combi, T.I. Gombosi, A.F. Nagy, D.L. DeZeeuw, K.G. Powell. *On Europa's Magnetospheric Interaction: An MHD Simulation of the E4 Flyby. J. Geophys. Res.* **104**, 19983-19992, 1999.
- 4) Kabin, K., K.C. Hansen, T.I. Gombosi, M.R. Combi, T.J. Linde, D.L. DeZeeuw, C.P.T. Groth, K.G. Powell, A.F. Nagy. *Global MHD Simulations of Space Plasma Environments: Heliosphere, Comets, Magnetospheres of Planets and Satellites. Astrophys. Space Sci.* **274**, 407-421, 2000.
- 5) Liu, Y., A.F. Nagy, K. Kabin, M.R. Combi, D.L. DeZeeuw, T.I. Gombosi, K.G. Powell. *Two-Species 3D MHD Simulation of Europa's Interaction with Jupiter's Magnetosphere. Geophys. Res. Lett.* **27**, 1791-1794, 2000.
- 6) Kabin, K., M.R. Combi, T.I. Gombosi, K.C. Hansen, K.G. Powell. *Io's Magnetospheric Interaction: An MHD Model with Day-Night Asymmetry. Planet. Space Sci.* **49**, 337-343, 2001.
- 7) Combi, M.R., T.I. Gombosi, K. Kabin. *Plasma Flow Past Cometary and Planetary Satellite Atmospheres, in Comparative Planetary Aeronomy, AGU Monograph Series (in press), 2002.*

Preliminary calculations using the kinetic DSMC model, given here, have been described at a number of conferences (Bauske and Combi 1998a&b, 1999). Although we would not describe our recent publication output from the current grant as inadequate, we do acknowledge that publication of a full paper documenting the model and giving first results has been hampered by a number of unfortunate non-technical problems. These include loss of a Co-I to industry because of uncertainty in continued funding and a delayed start of a graduate student because of personal circumstances. A new student, Mr. Valeriy Tenishev, has come to Michigan with a M.S. degree, having significant experience with DSMC methods and related programming. He has been coming-up-to-speed in learning the DSMC code. In the remainder of the current grant year we will complete a study running all neutral species in the DSMC model and adopting the ion flow from our published MHD models, with the goal of submitting a paper for publication.

Impact of This Work. The combination of modeling tools at our disposal provides us with a unique capability to address all the important components of a coupled system of neutral gas molecules, radicals and atoms, plasma ions and electrons and electromagnetic fields. Most modeling efforts concentrate on one aspect of the problem, and do that part extremely well. However, most so-called “self-consistent” treatments of one aspect of the problem, no matter how well-done, are forced to make rough assumptions about one of the other fundamentally important parts of the problem.

Copies of all of the refereed publications are attached as an appendix to this report. A summary of the kinetic ion and neutral DSMC modeling effort (Bauske & Combi, 1998a&b, 1999) follows.

Kinetic Ion-Neutral DSMC Model. Important processes in thin tenuous atmospheres, such as that of those around Jupiter’s satellites, like Io, and the upper atmospheres and ionospheres of the terrestrial planets, work on various energy and rate scales. In order to merge the many local processes into a global three-dimensional picture, a model is needed, which can include these processes on a small spatial scale and which can diversify the different energy scales. At the same time there are disparate time scales for various collision and gyration rates. This is difficult with a continuum (hydrodynamic) model alone. In order to model acceleration processes an electrodynamic or PIC type model is need, but then there are difficulties to include the chemistry. Our hybrid approach is a way out of this situation.

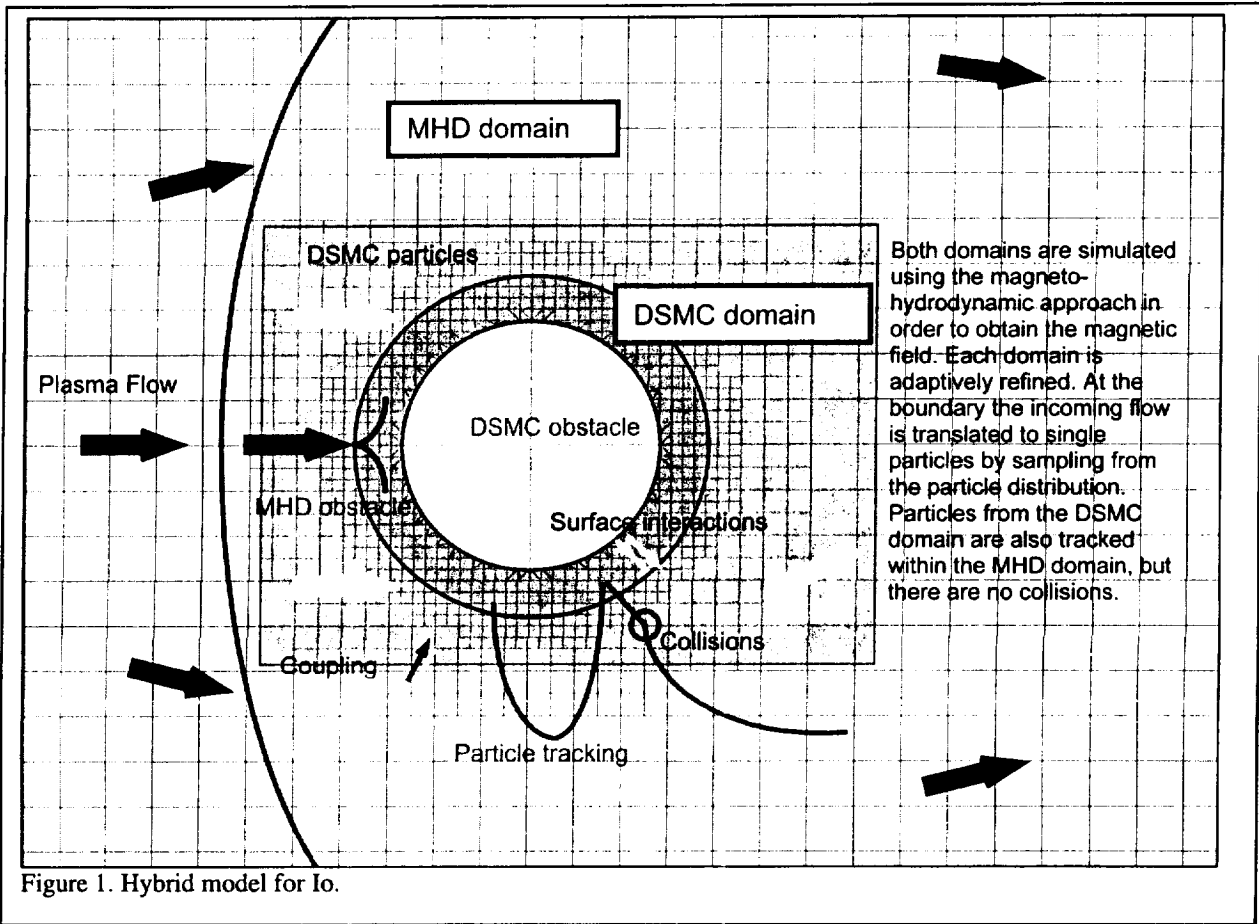
We have developed a 3D neutral and ion multi-species kinetic model, embedded in the multi-scale Cartesian grid of a 3D MHD code. The MHD part of this code has already been used in simulations of the mass-loaded flow of Jupiter's corotating magnetospheric plasma past Io (Combi et al., 1998) and other planetary applications (Bauske et al., 1998a,b; Kabin et al. 1999, 2000 & 2001; Liu et al. 2000). The DSMC part is specifically targeted towards analysis of kinetic processes as expected in tenuous atmospheres, from the ground outward to a distance of few times the body's radii.

The model couples the Direct Simulation Monte Carlo (DSMC) method (Bird, 1994) with a magnetohydrodynamics (MHD) (Powell et al., 1999). DSMC has a long history of application in areas as diverse as study of hydrodynamic shock structure, calculation of low-density, hypersonic flows around spacecraft and simulations of plasma reactors for

microelectronics manufacturing. Originally, the method was used to simulate the transition regime, where the mean free path of particles is too large for continuum hydrodynamics to be applicable. Because collisions are important, free molecular simulations are not appropriate. Therefore, individual particles are simulated as they move around within a grid, colliding with other particles and with solid objects. Macroscopic properties, such as density and temperature are computed by appropriate averaging of particle masses, locations, velocities, and internal energies. Momentum and energy exchanges with the surface allow for chemical reactions and sputtering effects. DSMC is based on the “rarefied-gas” assumption that over a short time interval or 'step' the molecular motion and the intermolecular collisions are uncoupled and therefore can be calculated independently. Molecules are moved over the distances appropriate for this time step, followed by the calculation of a representative set of collisions. The time step is small compared to the mean collision time and, the results are independent of its actual value.

Our model is divided into inner and outer domains. As shown in Figure 1, inner domain may contain a whole planetary obstacle (Io) and a fraction of its surrounding atmosphere / exosphere / plasma environment, e.g., a cube of a few Io radii. Both types of domains are simulated using MHD to obtain the magnetic field. In the inner domain, we embed the multi-species DSMC model for detailed simulations of neutral and plasma chemistry and energetics and surface interactions. An adaptively refined unstructured grid gives high resolution in all areas of interest. Each domain contains cells of various sizes to match specific local requirements. The MHD part can have high resolution at a planetary bow shock, while the DSMC part is able to simulate the outflow of hot gases near a volcanic source. At domain boundaries, the MHD flow entering a DSMC domain is converted to individual particles by sampling from the given velocity distribution. The particle-tracking algorithm accounts for gravity, centripetal, Coriolis and electromagnetic forces. Particles are tracked through both domains, collisions, however, are only calculated within the DSMC domain.

Our approach is unique in several ways: (1) It is a new method to incorporate a microphysical perspective into the continuum calculations of magnetohydrodynamics. (2) It differs considerably from pure electromagnetic approaches like the Particle-In-Cell (PIC) method, because PIC codes usually neglect particle-particle and particle-boundary collisions, or include Coulomb collisions without chemistry (Winske and Omid, 1996). (3) Many applications of the DSMC method today are in dilute, but collisionally dominated particle regimes where the



particles have nearly thermal collision energies and the ionization ratio is very low. This is not the case for the tenuous atmospheres. Our model can also explore the gap between the collision dominated and the collision free regime in partially ionized plasmas. We extend the range of the DSMC method towards the higher particle energies usually encountered in planetary ionospheric and magnetospheric plasma environments (hundreds of eV/amu).

Lutisan (1995) compared several variants of the DSMC method and found the No Time Counter technique (NTC) of Bird (1994) and the Null-Collision technique (Koura, 1986 & 1989) to be among the fastest and most reliable ones. We chose the NTC method for its simplicity and its closeness to classic kinetic theory. In a DSMC cell of volume V_c each simulated molecule represents F_n real molecules. The probability P of collisions between two simulated molecules during the time interval Δt is equal to the ratio of the volume swept out by their total cross-sections σ_T moving at the relative speed g between them to the cell volume,

$$P = F_n \sigma_T g \Delta t / V_c.$$

The average number of simulated molecules is $N = nV_c/F_n$ where n is the density of the real molecules. P is generally a very small quantity. Therefore it is inefficient to calculate the full set of collisions by selecting all of the $N(N-1)/2$ simulation pairs and computing the collisions with this probability. The procedure can be made more efficient if only a fraction of the possible collision pairs is included and the resultant probability increased by dividing by this fraction. Efficiency is maximized if the fraction is such that the maximum probability becomes unity. Bird's NTC method for collisions of species p molecules with molecules of species q is that

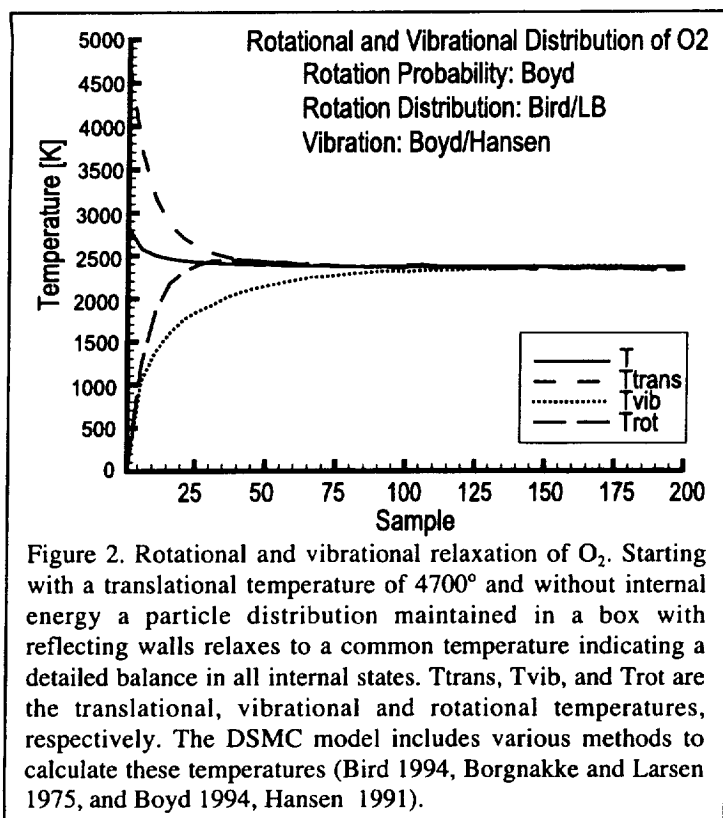
$$\frac{1}{2} N_p \bar{N}_q F_n (\sigma_T g)_{pq}^{\max} \Delta t / V_c$$

pairs are selected and the collisions are computed with probability

$$P = \frac{P}{P_{\max}} = \frac{\sigma_T g}{(\sigma_T g)_{pq}^{\max}}$$

where \bar{N}_q is the average number of species q simulation particles in the cell and $\sigma_T g$ is the product of cross section and relative velocity of the selected pair. Note that the rate of collisions is not affected by the value of $(\sigma_T g)_{pq}^{\max}$. This parameter is initially set to a large but reasonable value for this species combination and stored for each cell with the provision for it to be automatically updated if a larger value is encountered. After certain numbers of collisions, it is reset in order to account for time dependent changes in the species population.

In contrast to Bird, we allow a particle to undergo several changes of its internal energy per time step, thus allowing for fewer particles per cell and larger time steps where necessary. We added functionality beyond the basic algorithms suggested by Bird (1994) to account for chemical reactions and collisions with large inelastic cross sections. Apart from higher energies than in usual DSMC calculations, we also face the difficulty to simulate regions with orders of magnitude differences in density and also the inclusion of a model chemistry, which contains a variety of different species including trace species. Our basic idea for solving these problems numerically is to use weighted species groups and a regularly spaced subgrid within each cell of the adaptive grid structure. Usually every particle in a simulation cell represents a fixed number of real particles. This leads to problems if one species is underrepresented since a large number of samples is necessary to get reasonable statistics for this species. A weighting method (e.g., see Serikov, 1991; Miller and Combi, 1994) artificially changes the species value in order to allow for more simulation particles and to keep the overall number computationally feasible.



collisions. It determines the number of selections and the acceptance of the collisional momentum, energy, and type-change for the higher weighted particle. Weighting is used to keep computationally reasonable numbers of simulation particles in different density regimes roughly equal by comparing particle weights to a cell weight (Combi, 1996). Particles with higher weights are replicated, and those with lower weights are deleted with a probability set by the ratio of the particle weight to the cell weight.

We have tested and included methods (Boyd, 1993 & 1994; Wysong and Wadsworth, 1998) to calculate the probability of internal energy redistribution during a collision based on the species combination, the individual collision energy, and the internal states of the participating particles. The particle-based approach is more reliable at high energies and low densities than methods that use constant or temperature-dependent probabilities. Reliable DSMC methods are required to reach equipartition of internal and translation energies under equilibrium conditions. This requirement is fulfilled in our methods, if constants of the underlying molecular models are properly calibrated. Figure 2 shows an example for rotational and vibrational relaxation of O_2 .

Our hybrid model specified for Io, includes species O , S , O_2 , S_2 , SO , SO_2 , SO_3 , and the corresponding ions. We account for $O^+(^4S)$, $O^+(^2D)$, $O^+(^2P)$, $S^+(^4S)$, $S^+(^2D)$, $S^+(^2P)$ as separate

We developed a weighting scheme consistent with the NTC method, which allows for trace species and conserves the overall momentum and energy balance on average. The number of selections for collisions is recalculated every time a species type-changing collision (reaction, ionization, etc.) occurs and the collision iteration proceeds as long as there are selections remaining. Our NTC variant employs a data structure, which allows fast addition and deletion of particles without needing to re-index all particles after

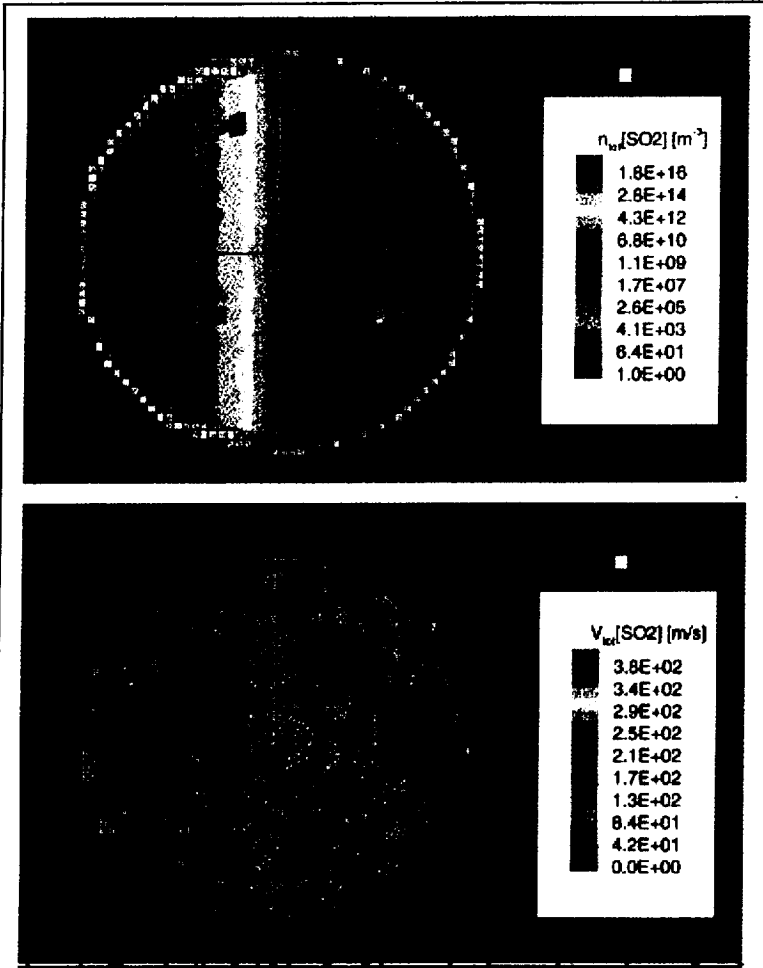


Figure 3. SO_2 densities in a sublimation and volcanic atmosphere around Io. The sun is to the left and a number of volcanic sources is distributed on Io's surface. Here, we show intermediate results of a DSMC, which started with a vacuum. After 1000 iterations the average densities in the lower altitudes of the atmosphere are established (compared to preceding results). The results for density and velocity are similar to the hydrodynamic results of Moreno et al., however the temperatures at high altitude are higher. This is similar to the results of Austin and Goldstein (2000) who found significant kinetic effects not too far above the surface. The linear cell size of our adaptive grid is 0.05 Io radii and each cell contains a subgrid with 64 cells to resolve the lower atmosphere.

species for photoionization and take care of the excess energies, which contribute to the electron energies for ionization, to the particle energies for dissociation, and to UV heating. Energy dependent solar photo rates and the solar photon fluxes are taken from Huebner et al. (1992). The plasma is currently assumed to be quasi-neutral, and as a first approximation the electron temperature is given by the scaled ion temperature—an improvement we plan to address.

Figure 3 shows intermediate results of a simulation for Io, where the evolution of an SO_2 sublimation and volcanic atmosphere without influences from the Io torus is studied. We simulated a region of 30 Io radii starting with a vacuum. Here we show SO_2 densities in a selected region around Io and on

Io's surface. After 1000 iterations using local time steps for each cell, the outflow of gas from the dayside of the planet and at several volcanoes on the day- and night-side almost filled the simulation region, but a state of equilibrium is not yet established. However, from comparisons with previous steps we know that changes in the maximum density between succeeding iterations are small and decreasing close to the surface, while the remaining empty cells fill with

simulation particles, and average values of variables such as cell densities temperature and flow velocities are established.

Finally, the PI would like to gratefully acknowledge the Planetary Atmospheres program and the current and past program managers for their support for this work.

III. References

- Bauske, R. and M.R. Combi. *Eos Transactions, AGU, Eos Transactions, AGU*, **79**, S200, 1998a.
- Bauske, R. and M.R. Combi. *Eos Transactions, AGU*, **79**, F551, 1998b.
- Bauske, R. and M.R. Combi. The Interaction of Io's Plasma Environment with the Neutral Atmosphere: Direct Monte Carlo Simulation of Io's Atmosphere from the Ground to 30 R-Io. Presented at "Magnetospheres of the Outer Planets" Paris, France, 9-14 August, 1999.
- Bauske, R., M.R. Combi, J.T. Clarke. *Icarus* **142**, 106-115, 1999.
- Bird, G. A., *Molecular gas dynamics and the direct simulation of gas flows*, Oxford University Press, 1994.
- Borgnakke, C. and P. S. Larsen. *J. Comput. Phys.* **18**, 405, 1975.
- Boyd, I. D. *Phys. Fluids A*, **5**, 2278, 1993.
- Boyd, I. D. *Progr. Astronaut. Aeronaut.* **159**, 78, 1994.
- Combi, M.R. *Icarus* **123**, 207-226, 1996.
- Combi, M.R., K. Kabin, T.I. Gombosi, D.L. DeZeeuw, K.G. Powell. *J. Geophys. Res.* **103**, 9071-9081 1998.
- Combi, M.R., T.I. Gombosi, K. Kabin. Plasma Flow Past Cometary and Planetary Satellite Atmospheres, in *Comparative Planetary Aeronomy*, AGU Monograph Series (in press), 2002.
- Hansen, C. F., *AIAA paper* 91-0465, 1991.
- Huebner, W.F., J.J. Keady, and S.P. Lyon. *Astrophys. and Sp. Sci.* **195**, 1, 1992.
- Kabin, K. MHD Simulation of Magnetospheric Interaction of Planets and Satellites, Ph.D. Thesis, University of Michigan, 2000.
- Kabin, K., M.R. Combi, T.I. Gombosi, A.F. Nagy, D.L. DeZeeuw, and K.G. Powell. *J. Geophys. Res.* **104**, 19983-19992, 1999.
- Kabin, K., K.C. Hansen, T.I. Gombosi, M.R. Combi, T.J. Linde, D.L. DeZeeuw, C.P.T. Groth, K.G. Powell, A.F. Nagy. *Astrophys. Space Sci.* **274**, 407-421, 2000.

- Kabin, K., M.R. Combi, T.I. Gombosi, K.C. Hansen, K.G. Powell. *Planet. Space Sci.* **49**, 337-343, 2001.
- Koura, K., *Phys. Fluids*, 29, 3509, 1986.
- Koura, K., *Prog. Astronaut. Aeronaut.*, 117, 25, 1989.
- Liu, Y., A.F. Nagy, K. Kabin, M.R. Combi, D.L. DeZeeuw, T.I. Gombosi, K.G. Powell. *Geophys. Res. Lett.* **27**, 1791-1794, 2000.
- Lutisan, J. *Molecul. Sim.* **14**, 189, 1995.
- Miller, R.N. and M.R. Combi. *Geophys. Res. Lett.* **21**, 1735-1738, 1994.
- Powell, K.G., P.L. Roe, T.J. Linde, T.I. Gombosi, D.L. DeZeeuw. *J. Comp. Phys.* **154**, 284-309, 1999.
- Serikov, V. V., Rarefied Gas Dynamics, *Proceedings of the 17th Symposium of Rarefied Gas Dynamics, Aachen 1990*, ed. A. E. Beylich, VCH Verlagsgesellschaft, Weinheim, Germany, 1991.
- Winske, D., and N. Omidi. *J. Geophys. Res.* **101**, 17287, 1996.
- Wysong, I. J. and D. C. Wadsworth. *Phys. Fluids* **10**, 2983, 1998.

IV. Appendix

Reprints of supported publications.